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Band gap energy and Urbach tail studies of amorphous SiO_x and V_2O_5 thin films

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Abstract : The optical properties of amorphous SiO_x thin films (140 to 220 nm thick) and V_2O_5 thin films (190 to 350 nm thick) prepared by electron beam evaporation technique at 300 K and 10^{-3} Pa are investigated in the wavelength range 350–900 nm. The results are analysed assuming optical absorption by indirect transitions. A systematic reduction of the optical band gap energy and a decrease in the width of the band-tail region is observed with increasing film thickness.

Keywords : Urbach tail, amorphous SiO_x and V_2O_5, ultraviolet and visible spectra

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For the last several decades, varieties of developed modern techniques and methods based on the interaction of light with matter (such as reflection, transmission, absorption, scattering or emission), have brought about a much better understanding of the atomic and electronic structure of both pure solids and solids with lattice defects [1,2].

Variations of absorption coefficient $\alpha(\omega)$ with absorbed photon energy $\hbar\omega$ which help us to determine band gap energy and Urbach tail are shown by the following relations.

The absorption coefficient $\alpha(\omega)$ is related to the transmission coefficient $T(\omega)$ [3]

$$\alpha(\omega) = \frac{2.303}{d} \log_{10}\{1/T(\omega)\}, \tag{1}$$

where d is the film thickness.

In the high absorption parabolic band edge region, $\alpha(\omega)$ ($>10^6$ m^{-1}) can be expressed in a general form [4,5]

$$\alpha(\omega) = B(\hbar\omega - E_{opt})^m / \hbar\omega, \tag{2}$$

where the exponent m characterizes the transition process with values : 2, 3, 1/2 and 3/2 for indirect-allowed, indirect-forbidden, direct-allowed and direct-forbidden transitions respectively in the k-space, B is a constant, $\hbar$ is the Planck's constant, ω is the angular frequency of light used and E_{opt} is the optical band gap energy. For $m = 2$ it offers the best fit for the optical absorption data in many oxides and chalcogenide glasses [2].

According to Davis-Mott model [6], the tails of localized defect states which originate from dangling bonds [6,7] should be rather narrow and should extend a few tenths of an electronvolt into the mobility gap. In the absorption band region 10^2 m^{-1} to 10^{-2} m^{-1} *i.e.*, in the tails of the localized defect states, the absorption coefficient $\alpha(\omega)$ is described by the empirical exponential Urbach rule given by [2,4].

$$\alpha(\omega) = \alpha_0 \exp(\hbar\omega / E_e), \tag{3}$$

where E_e is the width of the tails of localized defect states and α_0 is a constant. Eq. (3) is applied for many amorphous materials [2,4].

SiO_x is amorphous material of variable composition and structure [8]. V_2O_5 is also amorphous. The composition and structure of films depend on the deposition parameters such as film thickness, deposition rate, pressure and temperature of the substrate.

Band gap energy and Urbach tail of SiO_x ($0 < x < 2$) and V_2O_5 amorphous thin films are reported in this paper. The influence of film thickness on the optical properties is also discussed.

SiO_x films (140 nm, 180 nm, 220 nm thick) and V_2O_5 films (190 nm, 240 nm, 350 nm thick) were deposited by evaporating SiO (Union Carbide Ltd.) and V_2O_5 (Aldrich Chemical Company, Inc. USA) powders on clean Corning 7059 alkali-free borosilicate glass substrates held at 300 K and 10^{-3} Pa pressure in an Edwards coating plant having electron beam heating facilities. The electron beam heating system consists of a six-hearth turret with rotary drive, an electron beam gun mounted on a baffle plate, cermet hearths and tungsten emitter. A power supply unit capable of supplying 0–6 KV and 0–500 mA is furnished with HT voltage and emission current meters and variable transformers for control. By raising the cermet support by a spacer, the electron beam can be focussed on the cermet hearths containing the sample materials for evaporation.

The SiO_x and V_2O_5 film thickness were measured using a multiple beam interferometry technique. Deposition rate 5 nm sec^{-1} was used in the present work.

The optical transmission measurements of SiO_x and V_2O_5 thin films in the wavelength range 350–900 nm were carried out using double beam spectrophotometer. Absorption coefficient $\alpha(\omega)$ calculated directly from the transmission coefficient $T(\omega)$ and film thickness using the relation (1). The structures of SiO_x and V_2O_5 thin films were studied using the X-ray glancing angle technique.

X-ray investigations at 300 K have been carried out for the specimens of SiO_x and V_2O_5 materials and typical diffractograms showed the absence of peaks, which reveal that SiO_x and V_2O_5 films possessed amorphous structure.

The ultraviolet and visible transmission spectra, $[\alpha(\omega)\hbar\omega]^{1/2}$ *vs* $\hbar\omega$ and ln α *vs* $\hbar\omega$ plots of SiO_x films of different thickness are shown in Figures 1–3 respectively. The data of V_2O_5 samples of different thickness behave similarly. The curves of Figure 2 have well

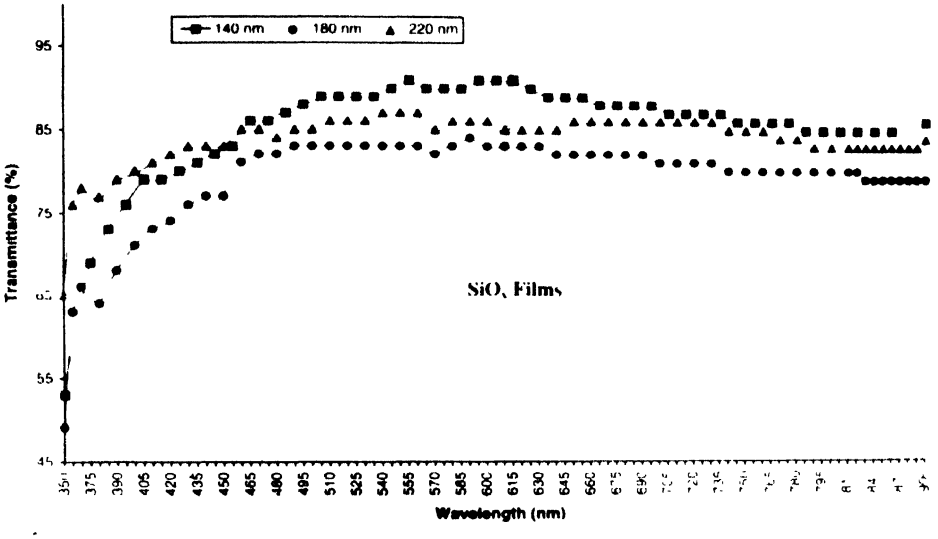

Figure 1. UV and visible spectra for the SiO_x films of different thickness

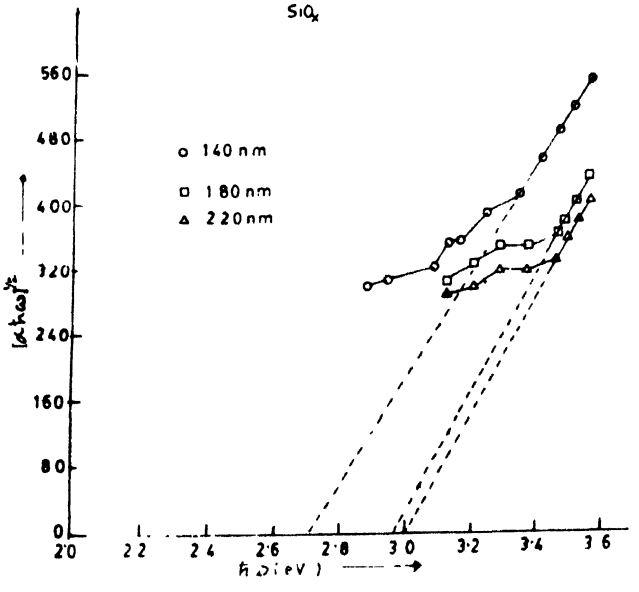

Figure 2. $[\alpha\hbar\omega]^{1/2}$ *versus* $\hbar\omega$ graphs of SiO_x films of different thickness.

defined linear regions. This confirms that eq. (2) for $m = 2$ is obeyed in the present work. Values of B and E_{opt} were calculated from the curves of Figure 2 and are recorded in Table 1.

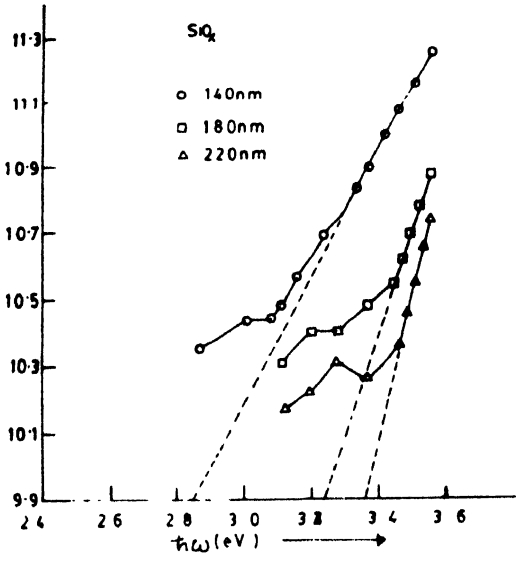

Figure 3. ln α *versus* $\hbar\omega$ graphs of SiO_x films of different thickness.

Table 1. Values of E_{opt}, B and E_e.

Film	Film thickness (nm)	Band gap energy in eV	Values of $B \times 10^5$ cm^{-1} eV^{-1}	Band tail energy in eV
	140	2.70	4.10	0.54
SiO_x	180	2.96	5.20	0.33
	220	3.00	4.80	0.25
	190	2.87	6.40	0.33
V_2O_5	240	2.90	4.50	0.27
	350	3.02	3.80	0.20

Figure 3 displays the exponential behaviour of the absorption band edge *via* eq. (3). The origin of the exponential behaviour of $\alpha(\omega)$ on photon energy in both crystalline and amorphous semiconductors is still uncertain. It may arise from fluctuation in the internal field associated with structural disorder in many amorphous solids or it is a consequence of electronic transitions between localized states in the band tails, the density of which is assumed to fall off exponentially with energy. Values of E_e calculated from the curves of Figure 3 are listed in Table 1. Values of E_{opt}, B and E_e of V_2O_5 samples of different thickness were calculated similarly and are recorded in Table 1.

It is observed from Table 1 that the value of E_{opt} increases slightly with increasing thickness of film while the value of E_e decreases with increasing thickness of film. This decrease in the value of E_e may be interpreted as follows.

At the beginning of the deposition process, some dangling bonds are likely to be created and these would be expected to act as structural defects which are responsible for the localized defect states in the material. As the thickness is increased a more homogeneous atomic network is built up thus reducing the proportion of defect states and the concentration of localized defect states [4].

Values of E_{opt} and E_e originate from the density of states at the band edges and from the density of localized defect states at the tails of the band edges [4] respectively. These values of amorphous SiO_x ($0 < x < 2$) and V_2O_5 thin films are in good agreement with the values in the literatures [2,3].

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